LA-UR- 04-6489

Approved for public release; distribution is unlimited.

Title: Comparison of Results from the MCNP Criticality Validation Suite Using ENDF/B-VI and Preliminary ENDF/B-VII Nuclear Data

Author(s): Russell D. Mosteller

Submitted to: International Conference on Nuclear Data for Science and Technology
Santa Fe, NM
September 26 - October 1, 2004

Comparison of Results from the MCNP™ Criticality Validation Suite Using ENDF/B-VI and Preliminary ENDF/B-VII Nuclear Data

Russell D. Mosteller

Diagnostics Applications Group (X-5), Applied Physics Division, Los Alamos National Laboratory
mosteller@lanl.gov

Abstract. The MCNP Criticality Validation Suite is a collection of 31 benchmarks taken from the *International Handbook of Evaluated Criticality Safety Benchmark Experiments*. MCNP5 calculations clearly demonstrate that, overall, nuclear data for a preliminary version of ENDF/B-VII produce better agreement with the benchmarks in the suite than do corresponding data from ENDF/B-VI. Additional calculations identify areas where improvements in the data still are needed.

INTRODUCTION

The final version of ENDF/B-VI (Release 8) was released in October 2001. A number of revisions to those nuclear data have been proposed for the preliminary version of ENDF/B-VII. To assess the reactivity impact of some of those revisions, calculations have been performed for the benchmarks in the MCNP Criticality Validation Suite[1] with the MCNP5 Monte Carlo code.[2]

CRITICALITY VALIDATION SUITE

The MCNP Criticality Validation Suite contains 31 benchmarks taken from the *International Handbook of Evaluated Criticality Safety Benchmark Experiments*.[3] As Table 1 indicates, those benchmarks encompass a wide variety of fissile isotopes, spectra, compositions, and configurations. The numbers in parentheses after the identifiers specify an individual case within a series.

TABLE 1. The MCNP Criticality Validation Suite.

	Fast Spectrum			Intermediate	Thermal Spectrum	
Fissile Material	**No Reflector**	**Heavy Reflector**	**Light Reflector**	**Various**	**Lattice of Fuel Pins**	**Solution**
^{233}U	Jezebel-233	Flattop-23	U233-MF-05 (2)	Falstaff (1)*	SB-2½	ORNL-11
HEU	Godiva Tinkertoy-2 (11)	Flattop-25	Godiver	UH_3 (6) Zeus (2)	SB-5	ORNL-10
IEU	IEU-MF-03	BIG TEN	IEU-MF-04	Zebra-8H†	IEU-CT-02 (2)	STACY (36)
LEU					B&W XI (2)	LEU-ST-02 (2)
Plutonium	Jezebel Jezebel-240 Pu Buttons (103)	Flattop-Pu THOR	Pu-MF-11	HISS/HPG†	PNL-33	PNL-2

* Extrapolated to critical † k_∞ measurement

Normal uranium is the reflector for all but one of the fast systems with heavy reflectors. The only exception is the thorium reflector for THOR. Water is the reflector for Godiver and Pu-MF-11, while beryllium and graphite are the reflectors for U233-MF-05 (2) and IEU-MF-04, respectively. Water is also the moderator for all of the lattices of fuel pins and solutions. All of the solution systems contain nitrate fuel except for LEU-ST-02 (2), which contains uranyl fluoride.

The MCNP Criticality Validation Suite was developed to assess the reactivity impact of future improvements to MCNP as well as changes to its associated nuclear data libraries. The suite is not an absolute indicator of the accuracy or reliability of a given nuclear data library (nor is it intended to be), but it can provide a general indication of the likely overall performance of the library. In addition, it can provide an early warning of unexpected or unintended consequences resulting from changes to nuclear data.

NUCLEAR DATA LIBRARIES

MCNP5 calculations were performed with two different combinations of nuclear data libraries. The first was a combination of the ENDF66[4] and ACTI[5] data libraries and the SAB2002 library of thermal scattering laws. This combination corresponds almost exactly to the final version of ENDF/B-VI and hereafter will be denoted as ENDF/B-VI. The second combination replaced the data for ^{237}Np, the uranium isotopes, and ^{239}Pu with data from the T16_2003 library, which is slated for general release in the near future. The most notable changes involved inelastic and elastic scattering cross sections, fission spectra, and the average number of neutrons emitted per fission.[6] In addition, these data were augmented by new sets of resonance parameters for ^{235}U in the unresolved resonance region and for ^{238}U in the resolved resonance region.[7] This latter combination will be referred to as Pre-ENDF/B-VII.

CALCULATIONS AND RESULTS

MCNP5 calculations were performed for the benchmarks in the Criticality Validation Suite using both combinations of libraries. With two exceptions, each of the calculations employed 550 generations of 10,000 neutrons each. In the two exceptions (SB-5 and Zebra-8H), only 350 generations were employed because those cases require substantially more computer time per history than the others. The results from the first 50 generations were omitted from the statistics for all cases, and therefore the results are based on 5,000,000 active histories (3,000,000 for SB-5 and Zebra-8H).

The results are presented in Table 2. Overall, the Pre-ENDF/B-VII results are clearly superior to those from ENDF/B-VI. In particular, the Pre-ENDF/B-VII value for k_{eff} differs from the benchmark value by one standard deviation or less for 19 of the 31 benchmarks and by two standard deviations or less for 26 of them. The corresponding numbers for ENDF/B-VI are 13 and 22, respectively.

Some of the improvements with the Pre-ENDF/B-VII data are particularly noteworthy. The most striking improvements occur for some of the benchmarks with fast spectra, especially the bare metal spheres (Jezebel-233, Godiva, and Jezebel) and BIG TEN. In addition, the agreement between the values of k_{eff} for the bare spheres and those for their Flattop counterparts reflected by normal uranium resolves a long-standing discrepancy. Similarly, the agreement between the calculated and benchmark values of k_{eff} for the uranium and plutonium spheres reflected by water (Godiver and Pu-MF-11, respectively) improves significantly.

The improvement in the agreement for BAW XI (2) suggests that another longstanding discrepancy may finally be resolved. In the past, many production libraries incorporated an *ad hoc* adjustment to the ^{238}U resonance integral. However, it appears that the new resonance parameters for ^{238}U may eliminate the need for that adjustment.

Results for a few of the benchmarks do deteriorate when the Pre-ENDF/B-VII data are employed. Specifically, k_{eff} for SB-2½ is underpredicted by more than two standard deviations, while k_{eff} for IEU-MF-03 and IEU-MF-04 are significantly overpredicted. The value for PNL-33, a lattice of MOX fuel pins, is now overpredicted as well, and the overprediction for THOR is larger than with ENDF/B-VI. Given the excellent agreement for the other fast plutonium systems, the latter discrepancy suggests that the fast cross sections for thorium need to be revised.

RESULTS FOR OTHER BENCHMARKS

Although the Pre-ENDF/B-VII data produce very impressive improvements for many of the benchmarks in the Criticality Validation Suite, improvements still are needed in a number of areas. These areas include the intermediate energy range for ^{235}U, angular scattering distributions for deuterium, and fast cross sections for ^{237}Np.

TABLE 2. Results for Cases in the MCNP Criticality Validation Suite.

Type	Spectrum	Case	Benchmark k_{eff}	Calculated k_{eff}: Pre-ENDF/B-VII	Calculated k_{eff}: ENDF/B-VI
^{233}U	Fast	Jezebel-233	1.0000 ± 0.0010	0.9992 ± 0.0002	0.9931 ± 0.0002
	Fast	Flattop-23	1.0000 ± 0.0014	0.9986 ± 0.0003	1.0003 ± 0.0003
	Fast	U233-MF-05 (2)	1.0000 ± 0.0030	0.9966 ± 0.0003	0.9976 ± 0.0003
	Intermediate	Falstaff (1)	1.0000 ± 0.0083	0.9877 ± 0.0005	0.9894 ± 0.0005
	Thermal	SB-2½	1.0000 ± 0.0024	0.9948 ± 0.0005	0.9967 ± 0.0005
	Thermal	ORNL-11	1.0006 ± 0.0029	1.0005 ± 0.0002	0.9968 ± 0.0003
HEU	Fast	Godiva	1.0000 ± 0.0010	0.9993 ± 0.0003	0.9962 ± 0.0003
	Fast	Tinkertoy-2 (11)	1.0000 ± 0.0038	1.0004 ± 0.0003	0.9972 ± 0.0004
	Fast	Flattop-25	1.0000 ± 0.0030	1.0030 ± 0.0003	1.0024 ± 0.0003
	Fast	Godiver	0.9985 ± 0.0011	0.9975 ± 0.0003	0.9948 ± 0.0003
	Intermediate	UH_3 (6)	1.0000 ± 0.0047	0.9953 ± 0.0004	0.9914 ± 0.0003
	Intermediate	Zeus (2)	0.9997 ± 0.0008	0.9976 ± 0.0003	0.9942 ± 0.0003
	Thermal	SB-5	1.0015 ± 0.0028	0.9960 ± 0.0006	0.9963 ± 0.0005
	Thermal	ORNL-10	1.0015 ± 0.0026	0.9991 ± 0.0002	0.9992 ± 0.0002
IEU	Fast	IEU-MF-03	1.0000 ± 0.0017	1.0028 ± 0.0003	0.9987 ± 0.0003
	Fast	BIG TEN	0.9948 ± 0.0013	0.9941 ± 0.0002	1.0071 ± 0.0003
	Fast	IEU-MF-04	1.0000 ± 0.0030	1.0078 ± 0.0003	1.0038 ± 0.0003
	Intermediate	Zebra-8H	1.0300 ± 0.0025	1.0188 ± 0.0002	1.0405 ± 0.0002
	Thermal	IEU-CT-02 (3)	1.0017 ± 0.0044	1.0009 ± 0.0003	1.0007 ± 0.0003
	Thermal	STACY (36)	0.9988 ± 0.0013	0.9988 ± 0.0003	0.9988 ± 0.0003
LEU	Thermal	B&W XI (2)	1.0007 ± 0.0012	1.0000 ± 0.0003	0.9968 ± 0.0003
	Thermal	LEU-ST-02 (2)	1.0024 ± 0.0037	0.9967 ± 0.0003	0.9957 ± 0.0003
Pu	Fast	Jezebel	1.0000 ± 0.0020	1.0004 ± 0.0003	0.9975 ± 0.0003
	Fast	Jezebel-240	1.0000 ± 0.0020	1.0001 ± 0.0003	0.9979 ± 0.0003
	Fast	Pu Buttons (103)	1.0000 ± 0.0030	0.9986 ± 0.0003	0.9962 ± 0.0003
	Fast	Flattop-Pu	1.0000 ± 0.0030	1.0005 ± 0.0003	1.0013 ± 0.0003
	Fast	THOR	1.0000 ± 0.0006	1.0081 ± 0.0003	1.0062 ± 0.0003
	Fast	Pu-MF-11	1.0000 ± 0.0010	0.9986 ± 0.0003	0.9970 ± 0.0003
	Intermediate	HISS/HPG	1.0000 ± 0.0110	1.0110 ± 0.0003	1.0105 ± 0.0003
	Thermal	PNL-33	1.0024 ± 0.0021	1.0066 ± 0.0003	1.0029 ± 0.0003
	Thermal	PNL-2	1.0000 ± 0.0065	1.0036 ± 0.0005	1.0033 ± 0.0005

$\sigma < |\Delta k| \leq 2\sigma$ $|\Delta k| > 2\sigma$

Although the PRE-ENDF/B-VII result for Zeus (2) is an improvement relative to that from ENDF/B-VI, a more complex picture emerges when all four of the graphite-moderated Zeus experiments are examined. As shown in Figure 1, both libraries produce an energy-dependent bias in reactivity, with the Pre-ENDF/B-VII results being consistently higher than their ENDF/B-VI counterparts by approximately 0.003 Δk. In contrast, MCNP's ENDF/B-V library produces a small bias that is essentially constant.

ENDF/B-VI produces generally poor agreement for heavy-water benchmarks, as shown in Table 3. The Pre-ENDF/B-VII data produce marginal improvements, primarily because of the changes in the resonance parameters for ^{235}U. However, more substantial improvements are seen when the initial ENDF/B-VI cross

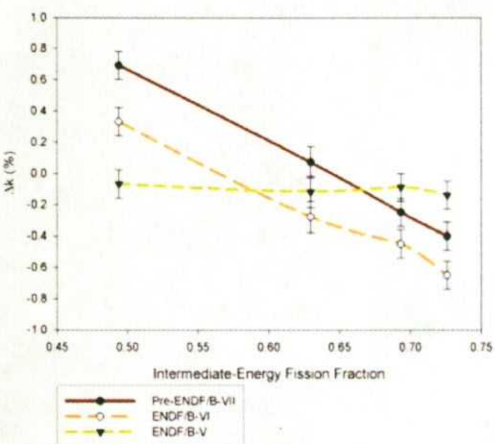

FIGURE 1. Results for Zeus Benchmarks.

TABLE 3. Results for Heavy-Water Solutions.

Benchmark	Case	Benchmark k_{eff}	Calculated k_{eff}: Pre-ENDF/B-VII + ENDF/B-VI.0 ^{2}D	Calculated k_{eff}: Pre-ENDF/B-VII	Calculated k_{eff}: ENDF/B-VI
Reflected Spheres (HEU-SOL-THERM-004)	1	1.0000 ± 0.0033	0.9948 ± 0.0004	0.9902 ± 0.0004	0.9839 ± 0.0004
	2	1.0000 ± 0.0036	0.9902 ± 0.0004	0.9846 ± 0.0004	0.9798 ± 0.0004
	3	1.0000 ± 0.0039	0.9962 ± 0.0004	0.9908 ± 0.0004	0.9861 ± 0.0004
	4	1.0000 ± 0.0046	0.9984 ± 0.0004	0.9937 ± 0.0005	0.9886 ± 0.0004
	5	1.0000 ± 0.0052	0.9969 ± 0.0004	0.9912 ± 0.0004	0.9871 ± 0.0004
	6	1.0000 ± 0.0059	0.9931 ± 0.0005	0.9876 ± 0.0004	0.9837 ± 0.0004
Unreflected Cylinders (HEU-SOL-THERM-020)	1	0.9966 ± 0.0116	1.0023 ± 0.0005	0.9902 ± 0.0005	0.9918 ± 0.0005
	2	0.9956 ± 0.0093	1.0079 ± 0.0005	0.9966 ± 0.0005	0.9967 ± 0.0005
	3	0.9957 ± 0.0079	1.0150 ± 0.0005	1.0046 ± 0.0005	1.0055 ± 0.0005
	4	0.9955 ± 0.0078	1.0136 ± 0.0005	1.0034 ± 0.0005	1.0029 ± 0.0005
	5	0.9959 ± 0.0077	1.0194 ± 0.0005	1.0114 ± 0.0005	1.0114 ± 0.0005

$\sigma < |\Delta k| \leq 2\sigma$ $\quad$ $|\Delta k| > 2\sigma$

sections for deuterium are used in place of the final ones. The principal difference between the two sets of cross sections is the angular distributions for elastic scattering.[8] While these results do not necessarily suggest that the initial deuterium cross sections should be retained, they do indicate that a further examination of the angular distributions would be appropriate.

In the neptunium-sphere benchmark, a central sphere of ^{237}Np is surrounded by HEU. As Table 4 indicates, ENDF/B-VI underpredicts k_{eff} for this benchmark by about 0.0125 Δk. Pre-ENDF/B-VII data produce better agreement but still leave k_{eff} underpredicted by approximately 1%.

TABLE 4. Results for the Neptunium-Sphere Benchmark (SPEC-MET-FAST-008).

Benchmark k_{eff}	Pre-ENDF/B-VII k_{eff}	ENDF/B-VI k_{eff}
1.0019 ± 0.0036	0.9922 ± 0.0003	0.9889 ± 0.0002

$|\Delta k| > 2\sigma$

CONCLUSIONS

Based on results for the MCNP Criticality Validation Suite, the Pre-ENDF/B-VII nuclear data produce substantially better overall results than do their ENDF/B-VI counterparts. The calculated values for k_{eff} for bare metal spheres and for an IEU cylinder reflected by normal uranium are in much better agreement with the benchmark values. In addition, the values of k_{eff} for the bare metal spheres are much more consistent with those for corresponding metal spheres reflected by normal uranium or water. In addition, a long-standing controversy about the need for an *ad hoc* adjustment to the ^{238}U resonance integral for thermal systems may finally be resolved.

On the other hand, improvements still are needed in a number of areas. Those areas include intermediate-energy cross sections for ^{235}U, angular distributions for elastic scattering in deuterium, and fast cross sections for ^{237}Np.

REFERENCES

1. Mosteller, R. D., "An Assessment of ENDF/B-VI Releases Using the MCNP Criticality Validation Suite," *Proc. PHYSOR 2004*, April 25-29, 2004, Chicago, IL, USA.
2. X-5 Monte Carlo Team, "MCNP — A General Monte Carlo N-Particle Transport Code, Version 5," Los Alamos National Laboratory report LA-UR-03-1987 (April 2003).
3. *International Handbook of Evaluated Criticality Safety Benchmark Experiments*, NEA/NSC/DOC(95)03, OECD Nuclear Energy Agency (2004 Edition).
4. Campbell, J. M., Frankle, S. C., and Little, R. C, "ENDF66: A Continuous-Energy Neutron Data Library for MCNP4C," *Proc. 12th Biennial Topl. Mtg. Radiation Protection and Shielding Div.*, Santa Fe, New Mexico, April 14-18, 2002 (2002).
5. Frankle, S. C., Reedy, R. C., and Young, P. G., "ACTI: An MCNP Data Library for Prompt Gamma-Ray Spectroscopy," *Proc. 12th Biennial Topl. Mtg. Radiation Protection and Shielding Div.*, Santa Fe, New Mexico, April 14-18, 2002 (2002).
6. MacFarlane, R. E., "Testing New Actinide Cross Sections Proposed for ENDF/B-VII," *Proc. Int. Conf. Nucl. Data Sci. Tech.*, Sep. 26 - Oct. 1, 2004, Santa Fe, NM, USA.
7. Leal, L. C., Derrien, H., and Larson, N. M., "Recent Cross Section Evaluations in the Resonance Region at the Oak Ridge National Laboratory," *Proc. Int. Conf. Nucl. Data Sci. Tech.*, Sep. 26 - Oct. 1, 2004, Santa Fe, NM, USA.
8. Campbell, J. M., personal communication (September 2004).